Structure Analysis of Jungle-gym-type gels by Brownian Dynamics Simulation(Poster session 1, New Frontiers in Colloidal Physics : A Bridge between Micro- and Macroscopic Concepts in Soft Matter)

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Abstract in Japanese:
化学ゲルの角度ポテンシャルの違う2つのモデルに関して、動径分布関数、構造因子およびループの分布を計算して、構造やダイナミクスを議論した。

1. Introduction

The network structure of gels [1,2] is important for determining the strength and other properties such as diffusion. Furukawa and coworkers [3-5] studied interesting jungle-gym type gels, analyzed by scanning microscopic light scattering (SMILS) and other methods.

We constructed two models[2] of gels, hard gel and soft gel, with different angle potentials. The structure and dynamics are analyzed for those two models.

2. Model and Method

Our model consists of triangular units, corresponding to trifunctional crosslinkers, and linear units, corresponding to oligomers. We perform Brownian dynamics simulation [6,7] using the Langevin equation:

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = -\frac{\partial U}{\partial \mathbf{r}_i} - \zeta \frac{d\mathbf{r}_i}{dt} + \mathbf{g}_i(t)$$

The second term of the right hand side is the effect of the viscosity, and the third term is the random force caused by solvent molecules.

2. Results and Discussion

We analyzed the loop structure and the distribution of crosslinking points.

The radial distribution of crosslinking points shows sharper peaks for hard gel than for soft gel.

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In Fig. 1, the number of closed loops in each system is shown. In soft gel, we find more loops than in hard gel. In particular, the small loops are more abundant for soft gel than for hard gel.

From other calculations, shrinking of clusters is found, and microgels form in early stage of the reaction in soft gel.

The details will be reported at the poster.

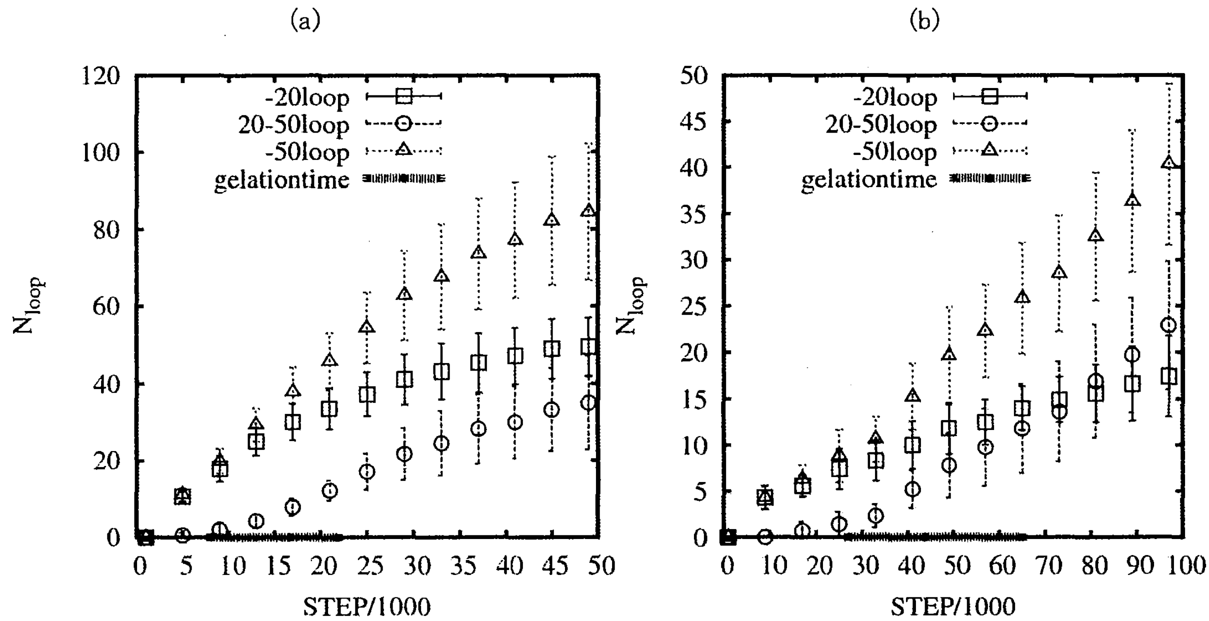

Fig. 1 The number of loops for soft gel (a) and hard gel (b), averaged over 10 samples. □ is for the small loops with $L_{size} \le 20$, ○ is for the large loops with $20 < L_{size} \le 50$, and □ is for all the loops with $L_{size} \le 50$. L_{size} is the number of particles constructing the loop.

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